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Prediction of the three-dimensional structure of the protein SaHPF and analysis of its molecular dynamics

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Abstract

© 2016, International Journal of Pharmacy and Technology. All rights reserved.SaHPF is the protein of gram-positive bacterium Staphylococcus aureus, which is causesa variety of diseases (pneumonia, meningitis, endocarditis, etc.), including nosocomial infections. SaHPF ishibernation-promoting factor, presumably interacts with the 30S subunit the ribosome and alters its conformation, and this results binding together of two ribosomes. Such ribosomal dimers do not perform protein synthesis, and this allows the cell to survive the unfavorable environmental conditions.The understanding of SaHPF-ribosome interaction mechanisms will allow to develop new antibacterial drugs. Protein structure was predicted using Robetta, Quark, I-Tasser, SWISS-MODEl and Phyre2 software, which used methods: homology, threading and ab initio. In total 24 protein models were built. Quality assessment of the obtained protein structures models was performed by Qmean program. Among the predicted structures, the most qualitative assessment was obtained model of the protein built in Robetta program, which builds the models by combining the methods of homology and ab initio. This model of the protein was analyzed by equilibrium molecular dynamics method in NAMD program, using Charmmforce field. The analysis of molecular dynamics trajectories using principal component and normal mode methods revealed a special mobility of the loop and the C-terminal domain of the protein, which may complicate the resolution of SaHPF structure by experimental methods (crystallography and NMR).

Keywords

In silico, Molecular dynamics, Prediction structure, Robetta, SaHPF, Staphylococcus aureus